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Investigation of non-Markovian kinetics of microscopic vortices in liquids

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Abstract

The non-Markovian kinetics of microscopic vortices in liquids is studied on the basis of the memory function formalism. Numerical calculations are carried out for liquid argon. The spectrum of vortex excitations, the relaxation times, the relaxation frequencies and the parameters of non-Markovity are obtained. Our theory coincides well with the molecular dynamics data.

1. Vortex motion is one of the most widespread motions of liquids in nature, determining the properties of both luminary and turbulent currents in fluids. The investigation of its properties is usually in terms of hydrodynamics [1–4], allowing one to explain a wide range of phenomena connected with macroscopic vortices. Studies of microscopic vortices (in a volume $\sim a^3$, where a is the interparticle distance) can be found in Refs. [5,6]. Vortices in microscopic small volumes of substances give essential contributions to the dynamic properties of liquids and dense gases.

The present Letter is devoted to the theoretical investigation of the physical properties of microscopic vortex motion in classical liquids and to the elucidation of the role of non-Markovian time effects in the appearance and disappearance of microscopic vortex structures.

2. Let us consider the instant value of the local velocity of particles in a liquid,

$$\boldsymbol{v}(\boldsymbol{r}) = V \sum_{j=1}^{N} \boldsymbol{v}_j \delta(\boldsymbol{r}_i - \boldsymbol{r}_j), \tag{1}$$

where V is the volume of the liquid, $\boldsymbol{r}_i$ is the radius-vector of the jth particle and $\delta(\boldsymbol{r})$ is the delta-function. We expand $\boldsymbol{v}(\boldsymbol{r})$ in a spatial Fourier integral,

$$\boldsymbol{v}(\boldsymbol{r}) = \frac{V}{(2\pi)^3} \int \mathrm{d}\boldsymbol{k}\, \boldsymbol{v}_k \exp(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}). \tag{2}$$

Here the Fourier components of the local velocity are

$$\boldsymbol{v}_k(t) = \sum_{j=1}^{N} \boldsymbol{v}_j(t) \exp\left[\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_j(t)\right] = \boldsymbol{v}_k^{\parallel}(t) + \boldsymbol{v}_k^{\perp}(t), \tag{3}$$

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